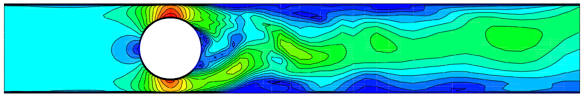
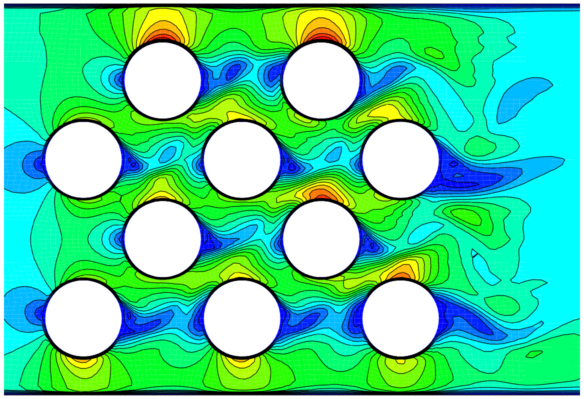
Challenges for CFD in Nuclear Applications

Texas A&M
UNIVERSITY
College Station, Texas, 77843
(409) 845-3211





Yassin Hassan
Texas A&M University

Advanced Simulation Workshop
December 14-16, 2005
Lawrence Livermore National Laboratory
Livermore, California

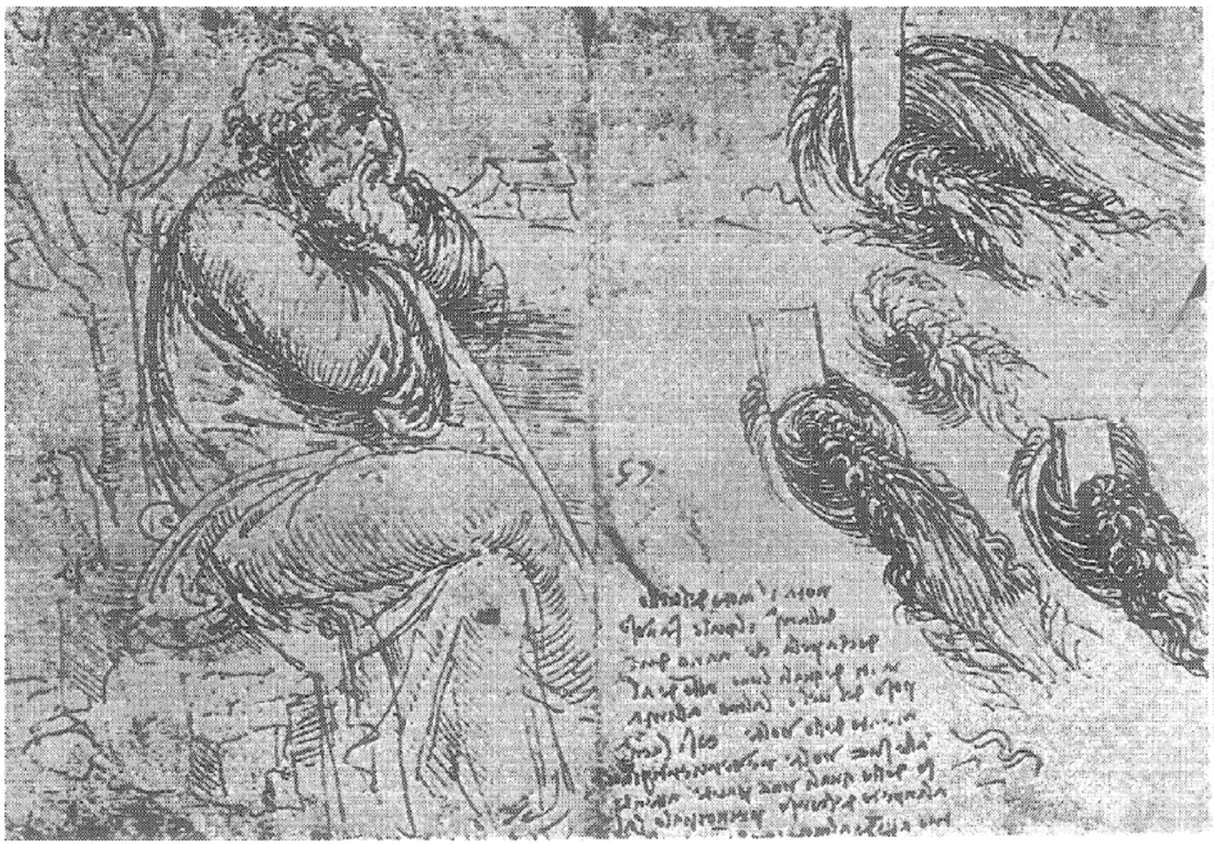
Motivation (Needs & Challenges)

- Unsteady flow predictions in complex structures is of both theoretical and practical importance.
- A database of such results will help improve the accuracy of numerical methods, near-wall models, and turbulence models.
- Design improvements will decrease down-time and increase lifetime of components.

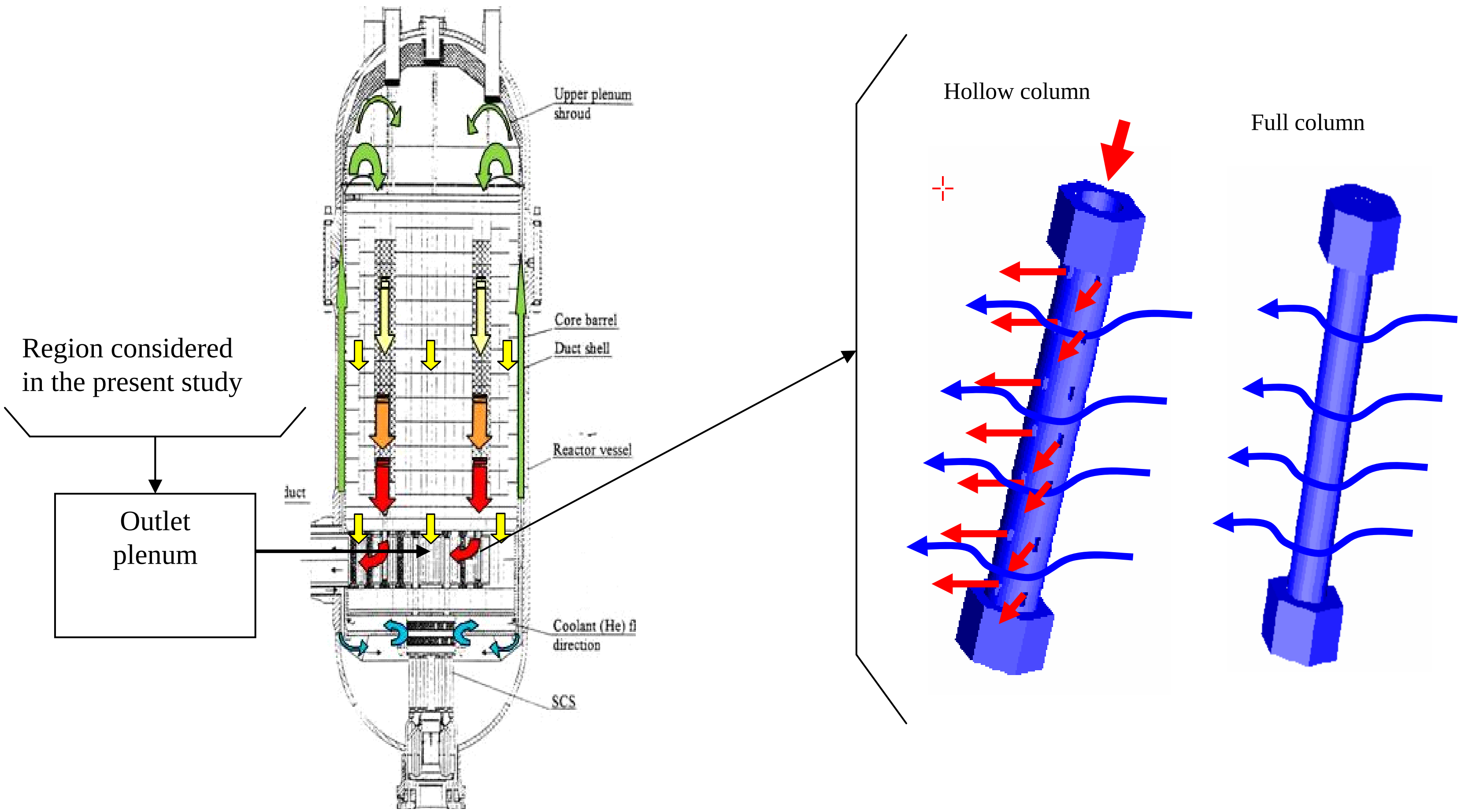
Objectives

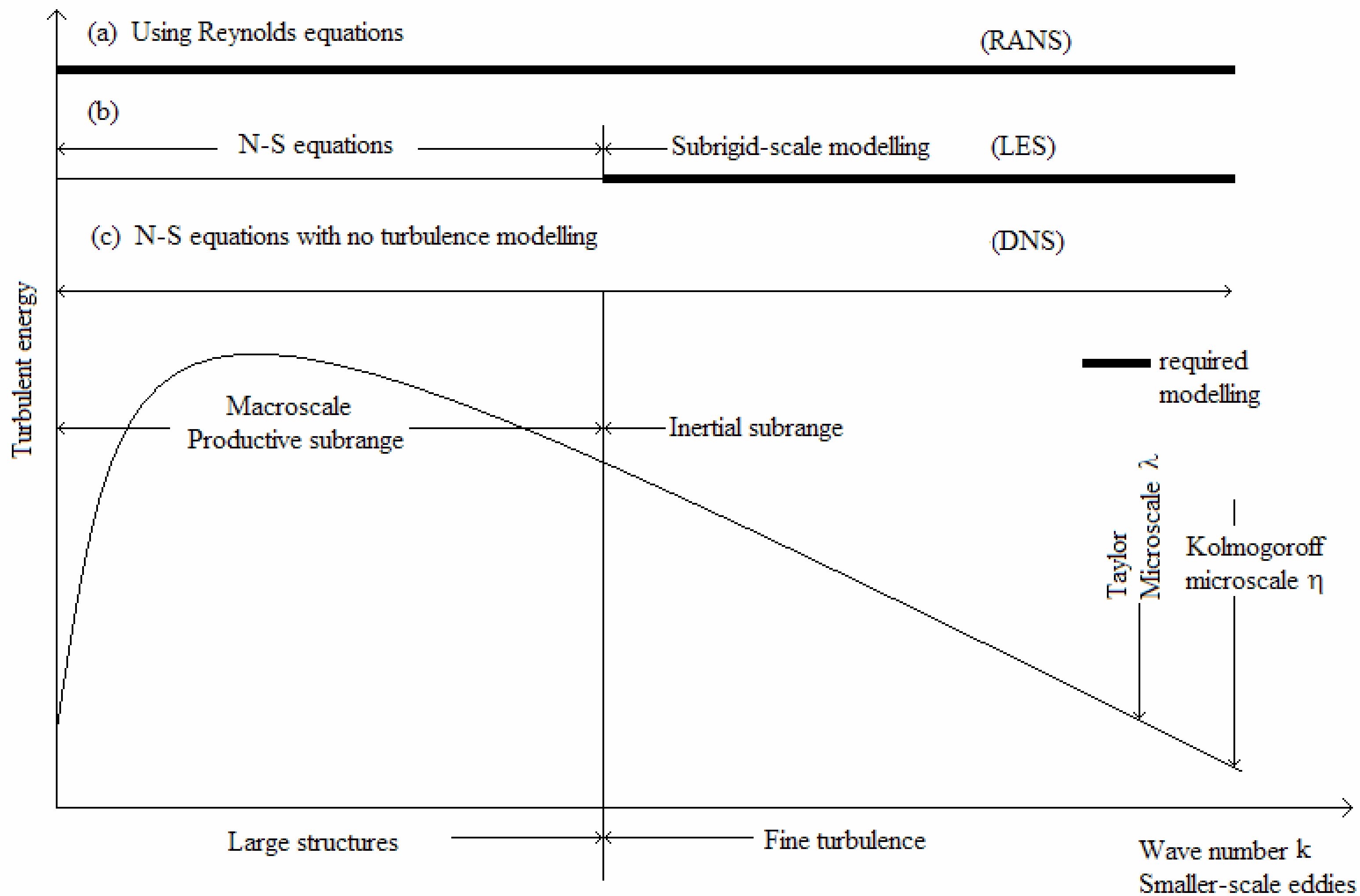
- To consider large eddy simulation in complex geometries.
- To evaluate closure and wall models and make appropriate modifications.
- To investigate the performance of these models by comparisons and visualizations.
- To perform tube bundle simulation as a practical application.

Leonardo da Vinci (1452-1519), his drawing and statement of coherent vortices around piers (The Royal Library, Windsor Castle)



•

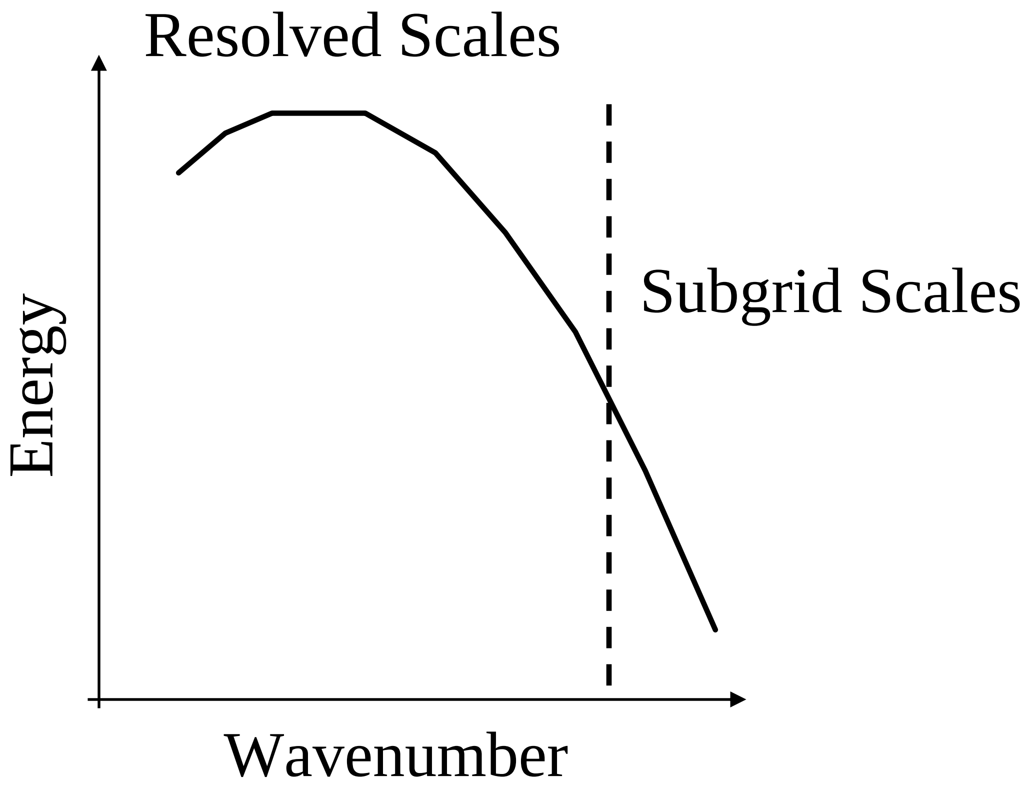

Region considered
in the present study
Outlet
plenum
Upper plenum
shroud
Core barrel
Duct shell
Reactor vessel
duct
Coolant (He) fl
direction
SCS
Hollow column
Full column



(a) Using Reynolds equations
(RANS)
(b)
N-S equations
Subrigid-scale modelling
(LES)
(c) N-S equations with no turbulence modelling
(DNS)
Turbulent energy
required modelling
Macroscale Productive subrange
Inertial subrange
Taylor Microscale λ
Kolmogoroff microscale η
Large structures
Fine turbulence
Wave number k
Smaller-scale eddies

Large Eddy Simulation

- Energy Spectrum



Large Eddy Simulation

- Large Eddy Simulation is a compromise between RANS and DNS methods.
- LES uses a spatial filtering technique where scales of turbulence above the grid size are resolved.
- Scales of turbulence below the grid size are modeled as dissipation (these scales are generally more universal).
- These are known as subgrid scale models.

Large Eddy Simulation

- Convolution filter used to separate instantaneous flow variables into resolved (large) and unresolved (subgrid) scales:

$$\bar{f}\left(x,t\right)=\int \bar{G}\left(x,x'\right) f\left(x',t\right)dx'$$

Continuity

$$\frac{\partial \bar{u}_i}{\partial x_i}=0$$

Momentum

$$\frac{\partial \bar{u}_i}{\partial t}+\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j}=-\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i}+\nu\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j}-\frac{\partial \tau_{ij}}{\partial x_j}$$

Subgrid Scale Modeling

- The goal of SGS modeling is to express the unresolved components in terms of the known values.
- The Smagorinsky model

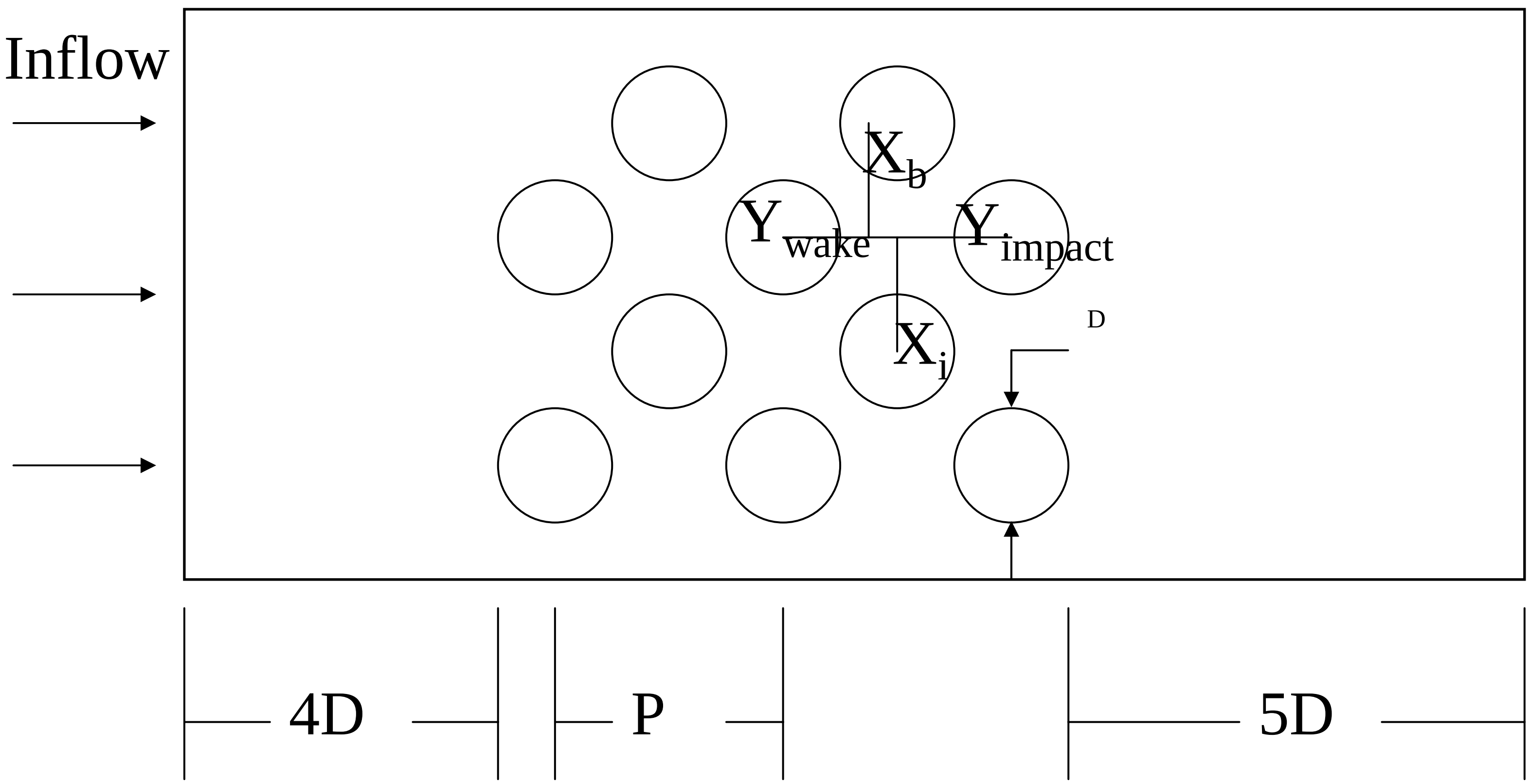
$$\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = -2\nu_T \bar{S}_{ij} \qquad \left|\bar{S}\right| = \left(2\bar{S}_{ij}\bar{S}_{ij}\right)^{1/2}$$

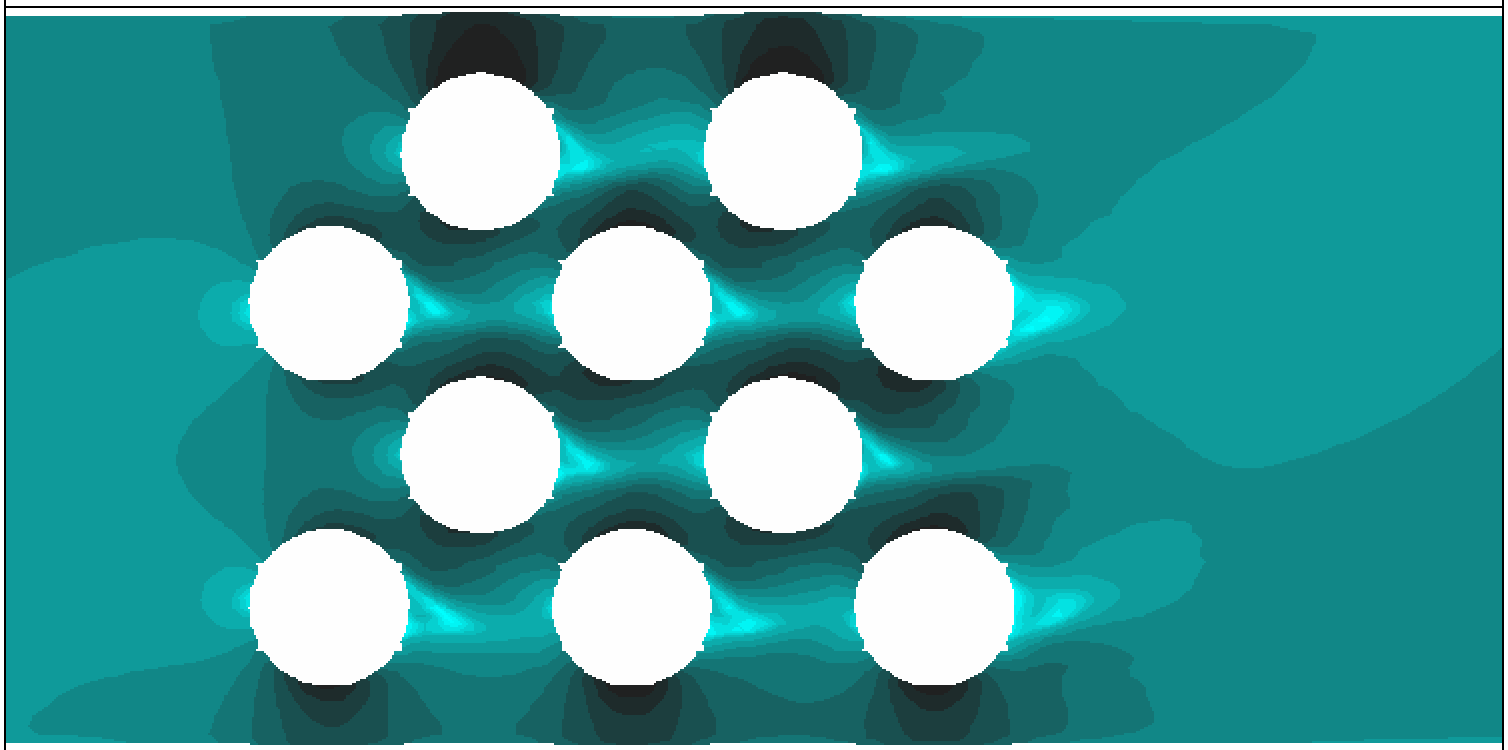
$$\nu_T = \left(C_S \Delta\right)^2 \left|\bar{S}\right| \qquad \bar{S}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)$$

Subgrid Scale Modeling

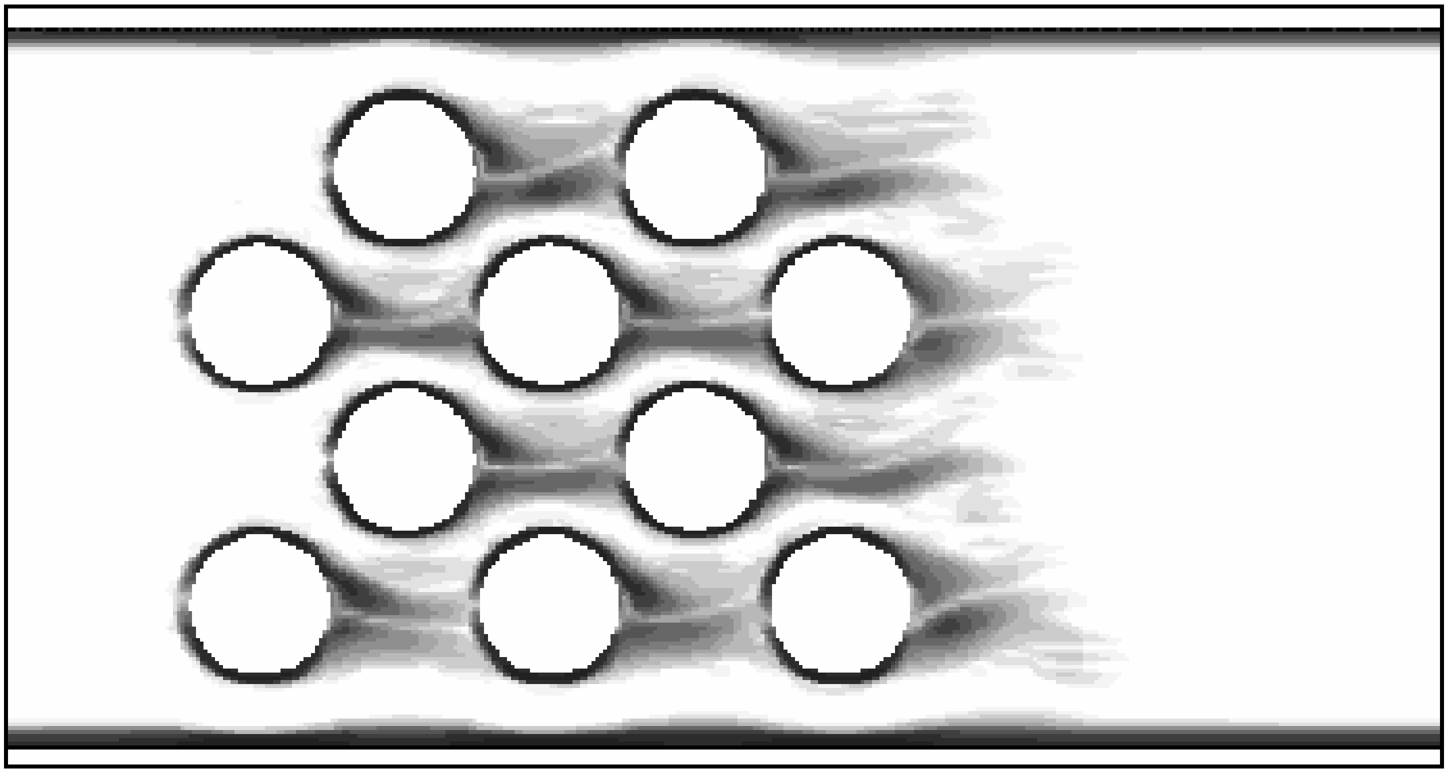
- Although the Smagorinsky model is the most widely used subgrid model, it has several drawbacks:
  - Incorrect behavior near walls (damping necessary)
  - Poor representation of Reynolds stresses (compared to DNS data)
  - Does not allow SGS energy backscatter
  - Model coefficient is flow dependent

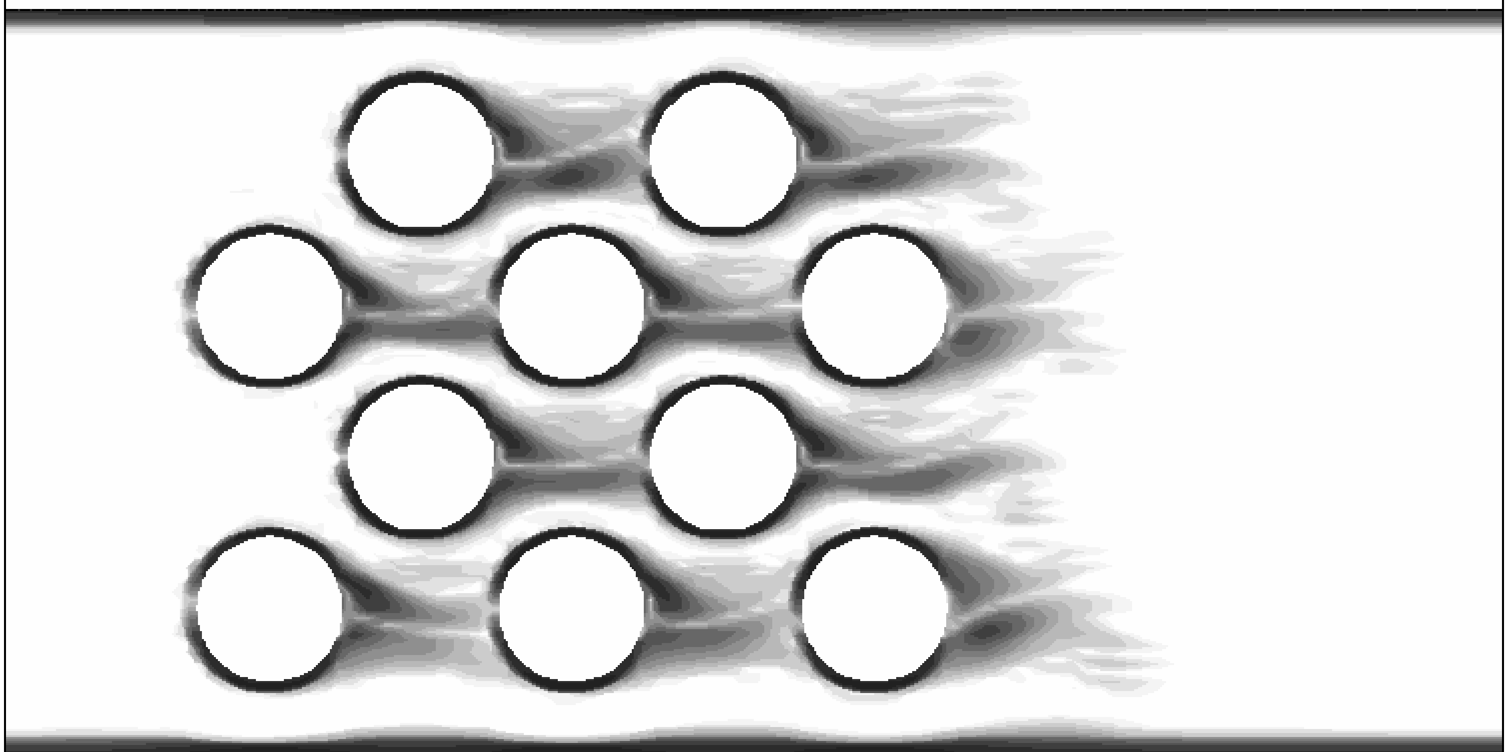
Tube Bundle Schematic





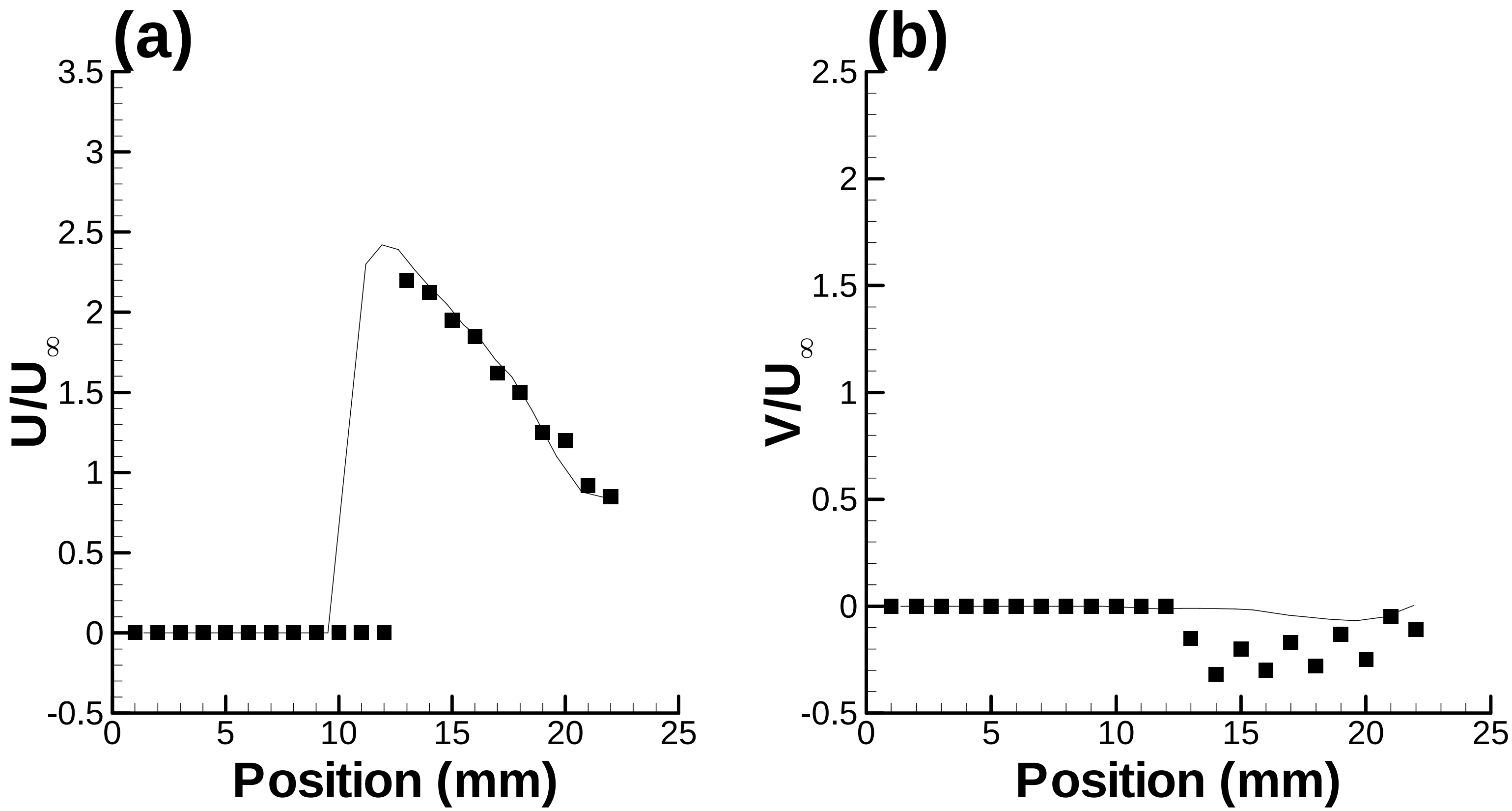
Velocity Magnitude



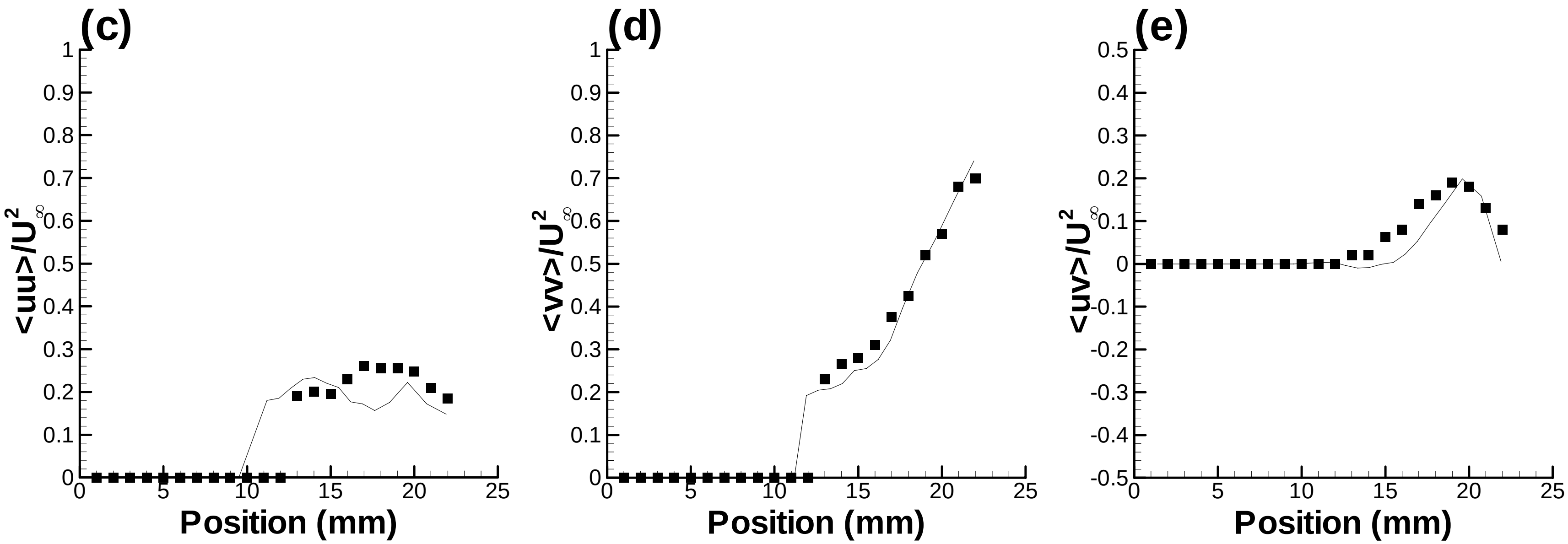


Vorticity Magnitude

Mean Velocity at X_i



Normal and Re Stress at X_i



Subcooled and Bubbly Flows Challenges

Complexity of multidimensional multiphase thermal hydraulic processes in nuclear components

Mass Conservation (field-j, phase-k)

$$\frac{\partial\left(\alpha_{jk}\rho_k\right)}{\partial t}+\nabla\bullet\left(\alpha_{jk}\rho_k\underline{\bar{v}}_{jk}\right)=\Gamma_{jk}+m'''_{jk}$$

Momentum Conservation (field-j, phase-k)

$$\frac{\partial\left(\alpha_{jk}\rho_k\underline{\bar{v}}_{jk}\right)}{\partial t}+\nabla\bullet\left(\alpha_{jk}\rho_k\underline{\bar{v}}_{jk}\underline{\bar{v}}_{jk}\right)+\nabla\left(\alpha_{jk}p_{jk}\right)$$

$$-\nabla\bullet\left(\alpha_{jk}\left[\underline{\underline{\bar{\tau}}}_{jk}+\underline{\underline{\tau}}^{T}_{jk}\right]\right)-\alpha_{jk}\rho_k\underline{g}-\underline{M}_{jk}-\underline{M}^{w}_{jk}=\Gamma_{jk}\underline{v}_{i}+m'''_{jk}\underline{v}_{jk}$$

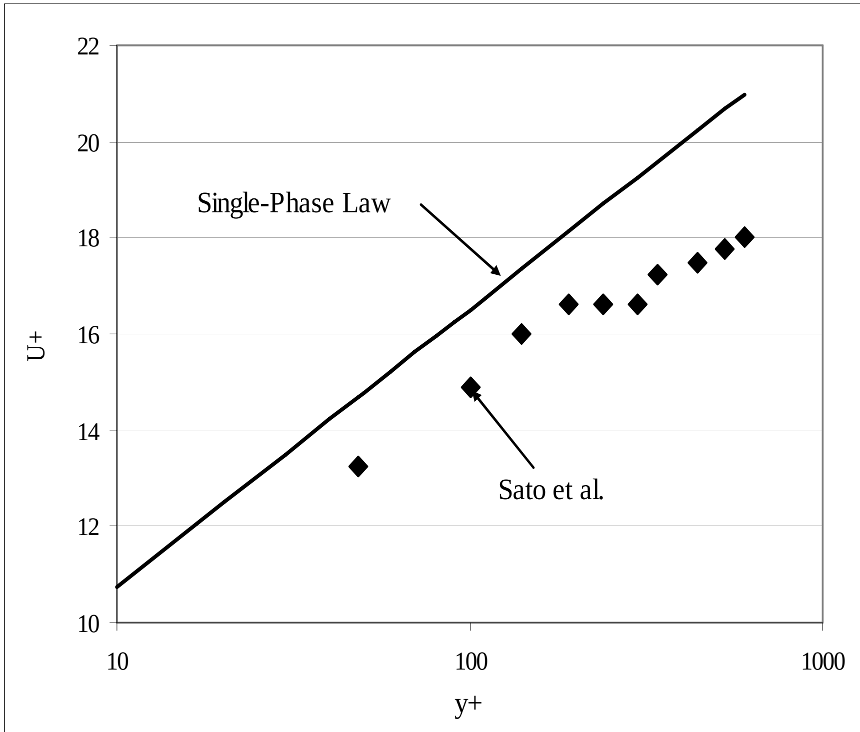
New Law of the wall for two-phase flow

$$U_{+} = \frac{1}{\kappa^{TP}} \ln\left(y_{+}\right) + B^{TP}$$

&TB 🖫 &SB ♌-1

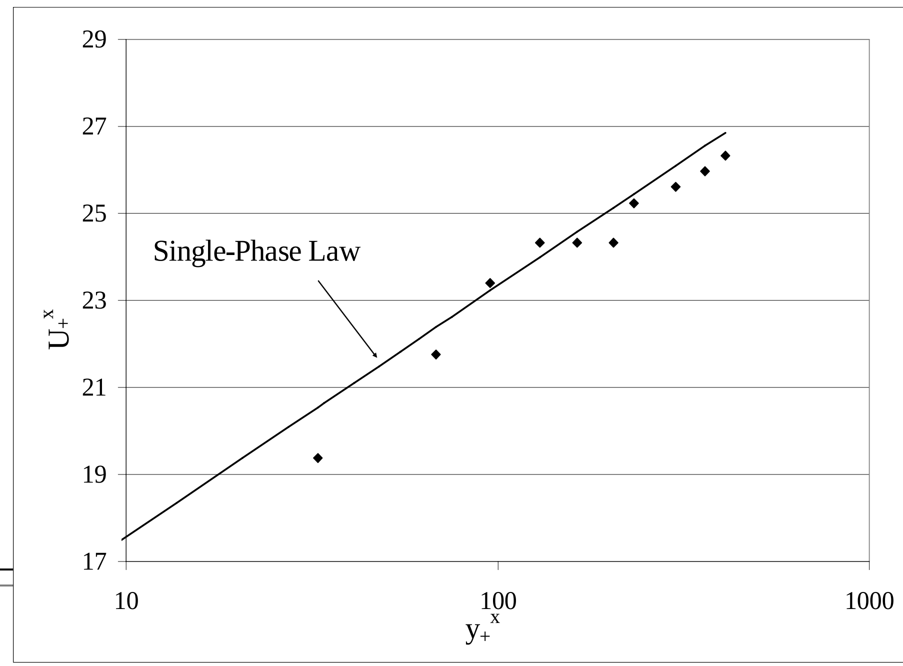
$$B^{TP} = y_{+}^{0}\left(\beta^{-1} - 1\right) - \ln\left(\beta\right) / \kappa^{SP}$$

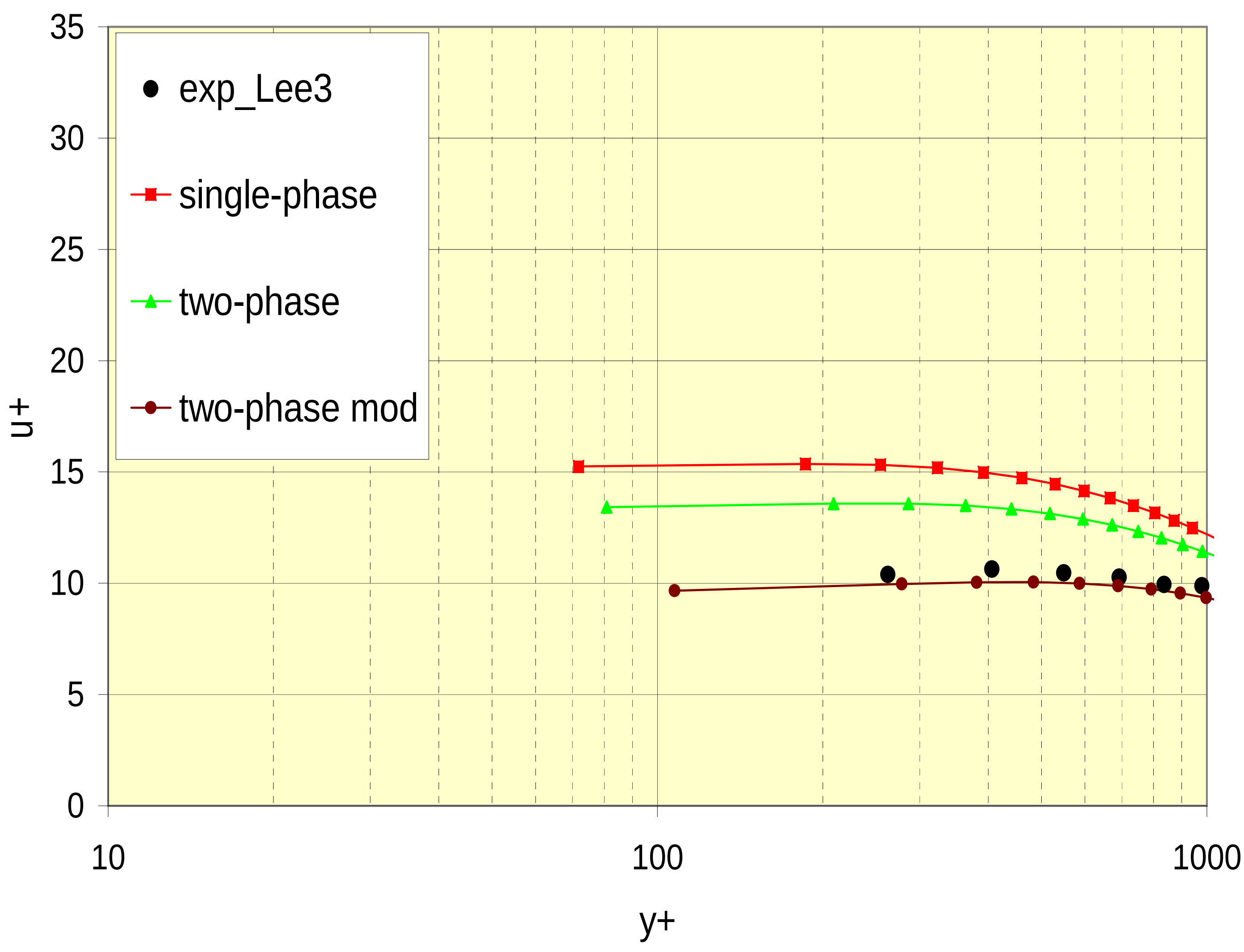
$$\beta = \left[\left(1 - \alpha_{\max}\right)\left(1 + \frac{\kappa_1 \alpha_{\max} \left|\mathbf{U}_r\right|}{\kappa^{SP} U_w^{TP}}\right)\right]^{-1}$$



With single-phase wall variables

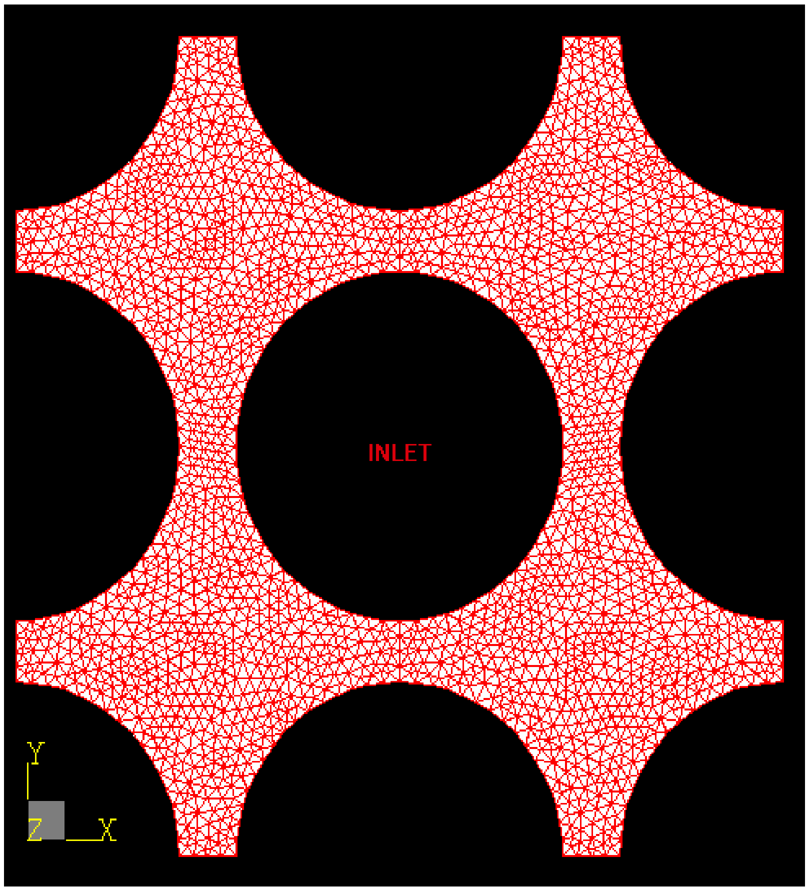
renormalized wall variables

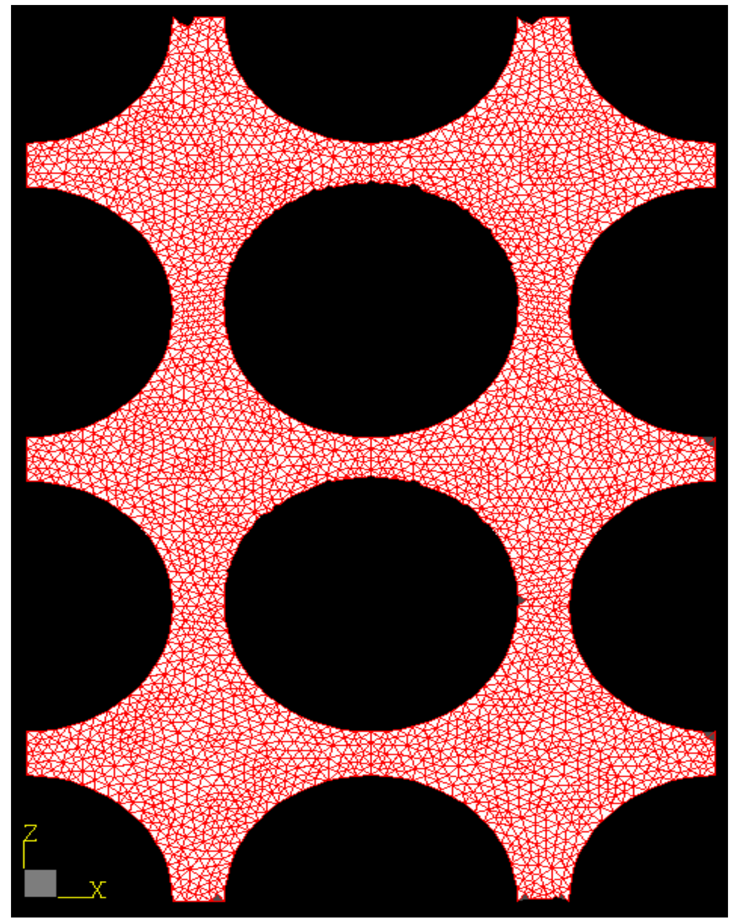




Non-dimensional axial velocity distribution in log layer for non-adiabatic conditions

Continued…





Continued…

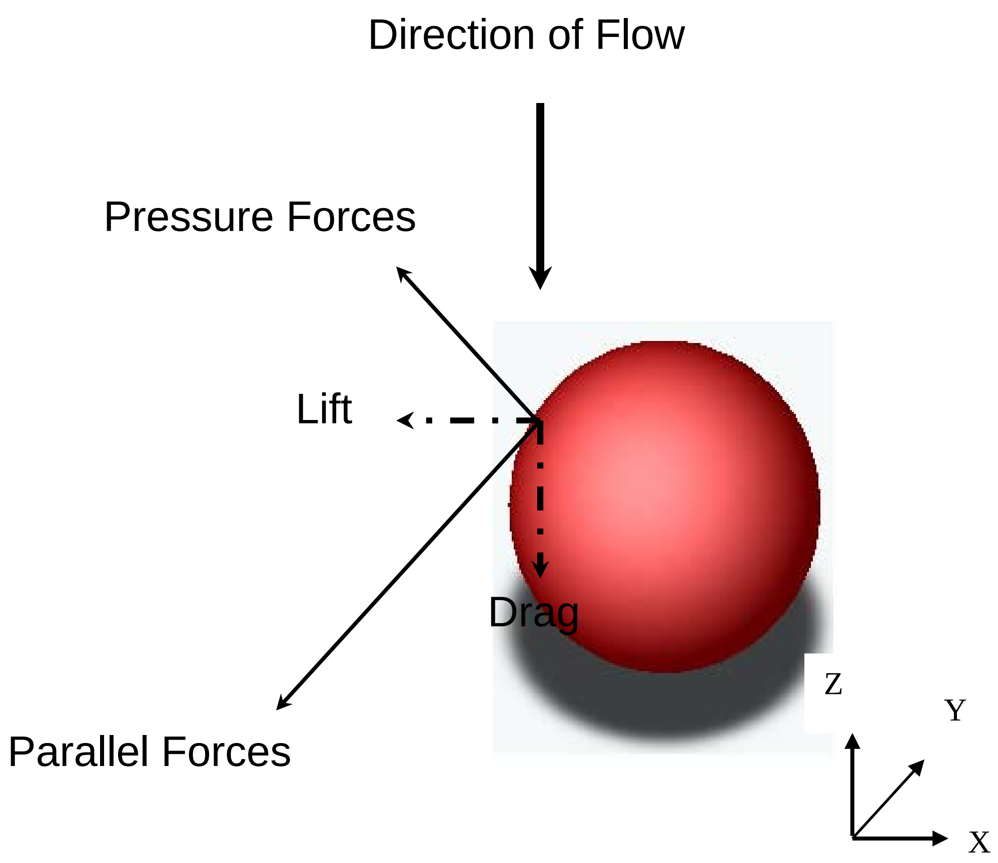
Mesh Statistics	
Number of nodes in surface mesh	82,827
Number of faces in surface mesh	165,594
CPU time for surface meshing	44.171 s
Number of elements in volume mesh	1,708,304
Number of nodes in volume mesh	332,759
Maximum element aspect ratio	6.14

- In the present study, 48-processor, 48GB distributed-shared-memory (DSM), system was used.
- This server called k2 is available at Texas A&M
- 4 CPU was utilized for Eddy Viscosity and Reynolds Stress turbulence models.

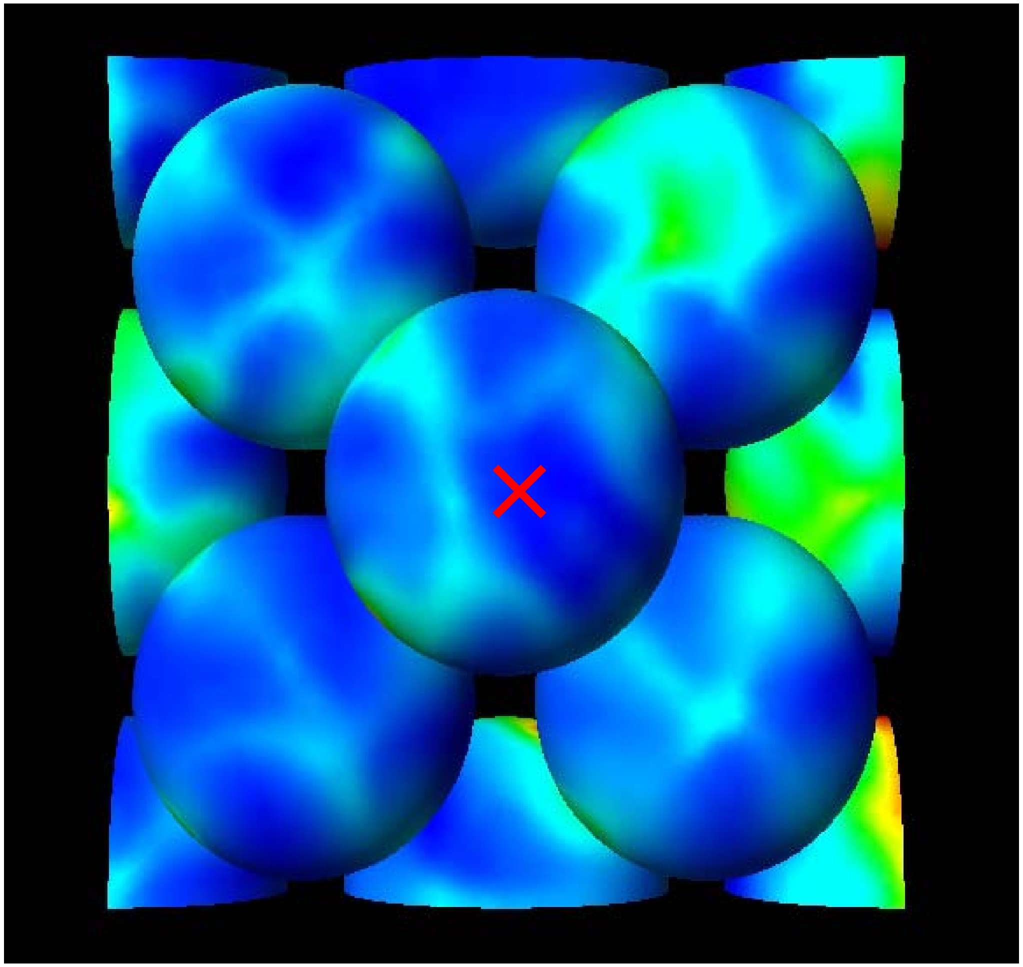
TURBULENCE MODELING

- DNS would require extremely fine grid at high Reynolds' number in order to capture small eddies.
- Therefore only RANS and LES turbulence modeling were used for the present study

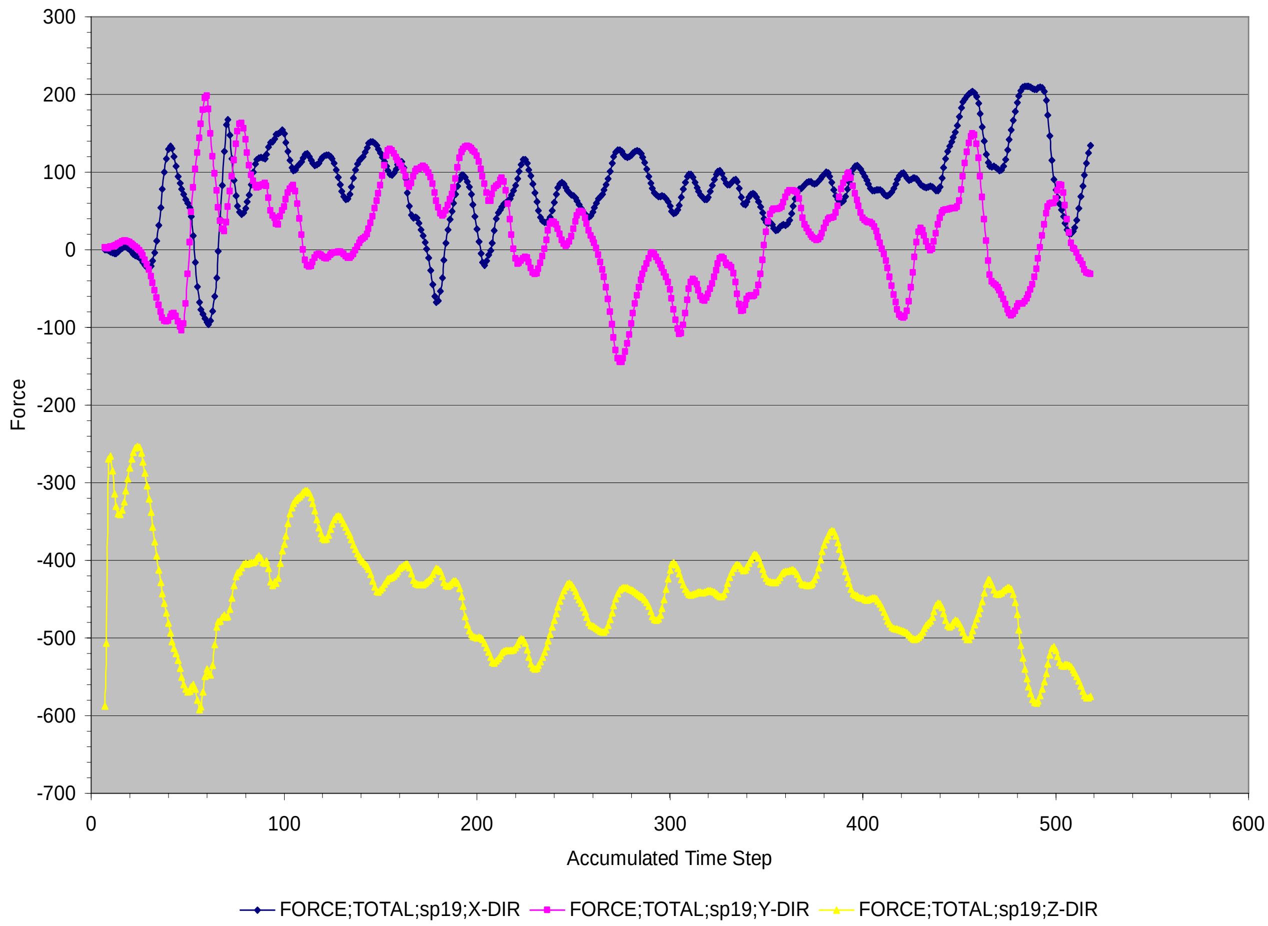
Drag and Lift Force Calculation



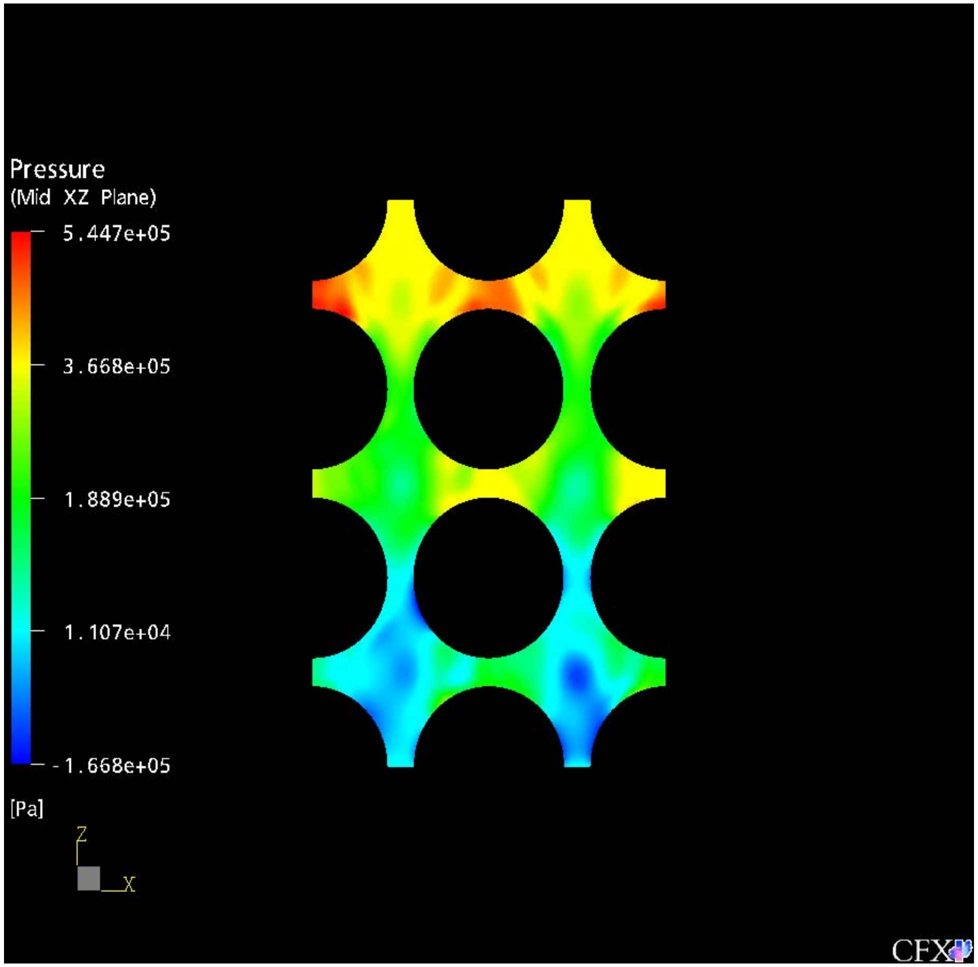
Location of Sphere Where Drag and Lift Forces Calculated



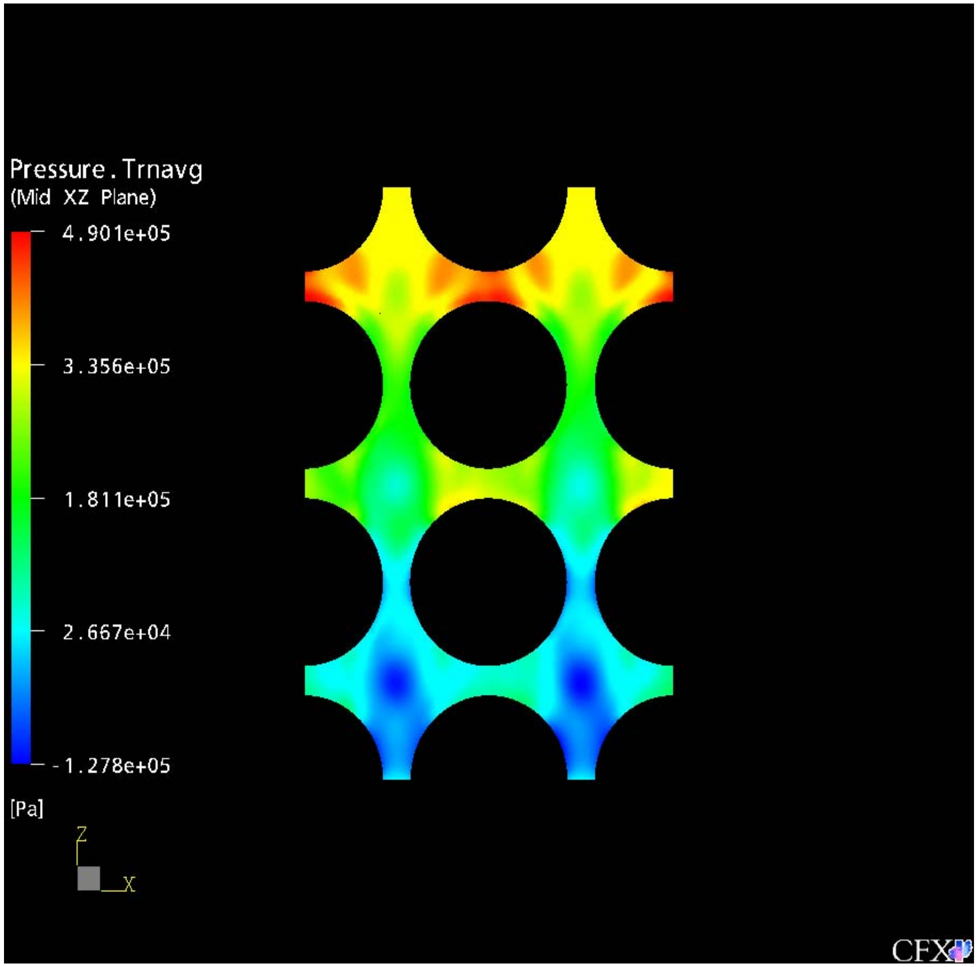
Total Drag and Lift Forces (LES)



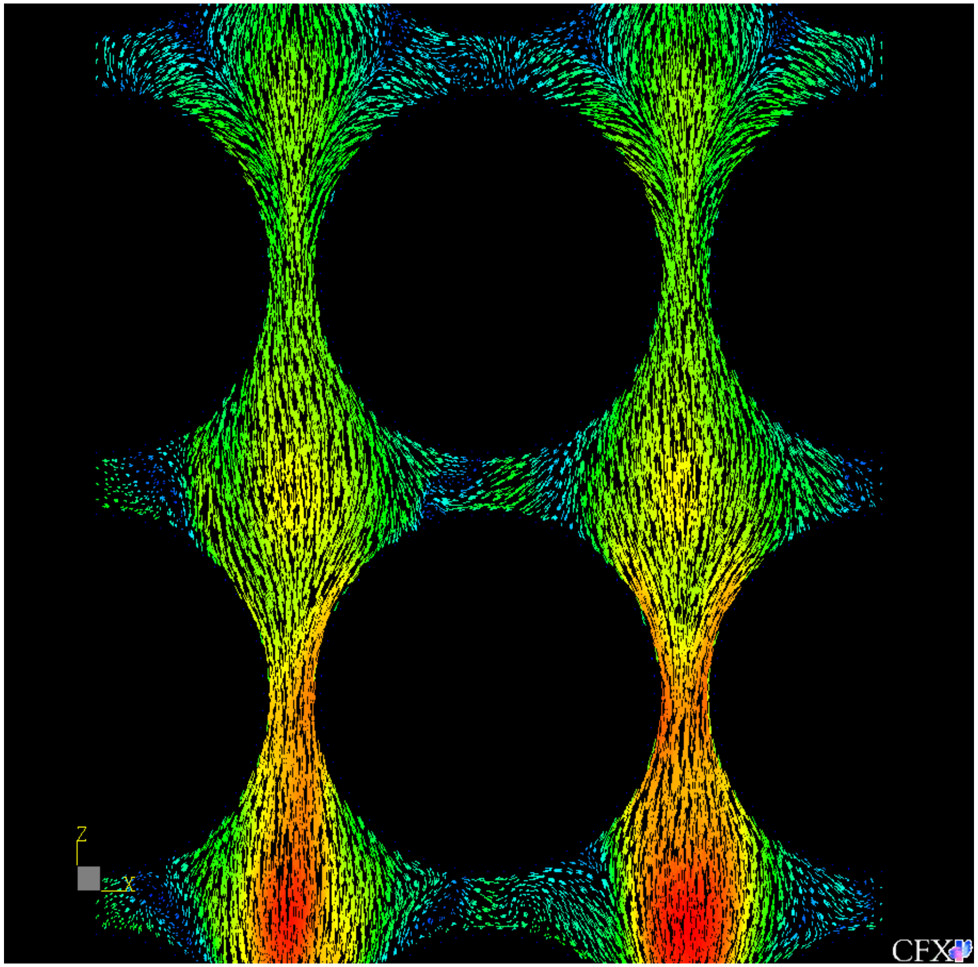
Pressure Distribution (Reynolds Stress Turbulence)



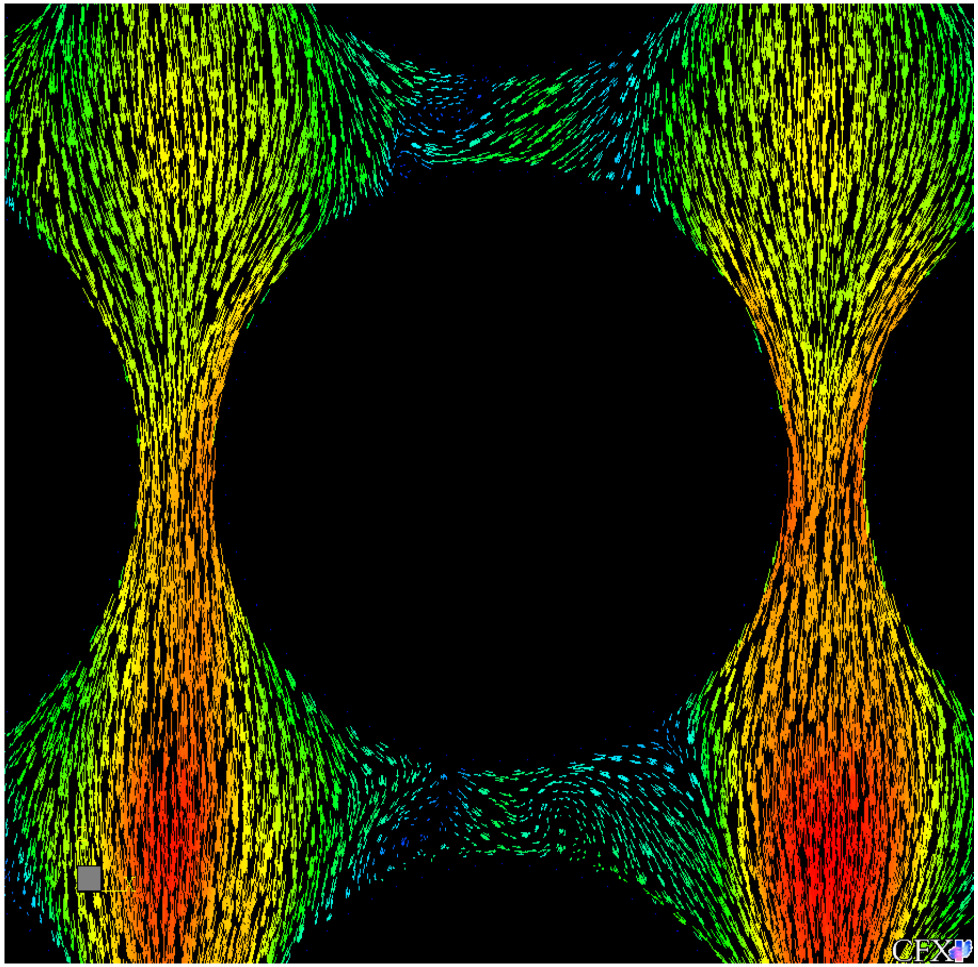
Average Pressure Distribution (LES)



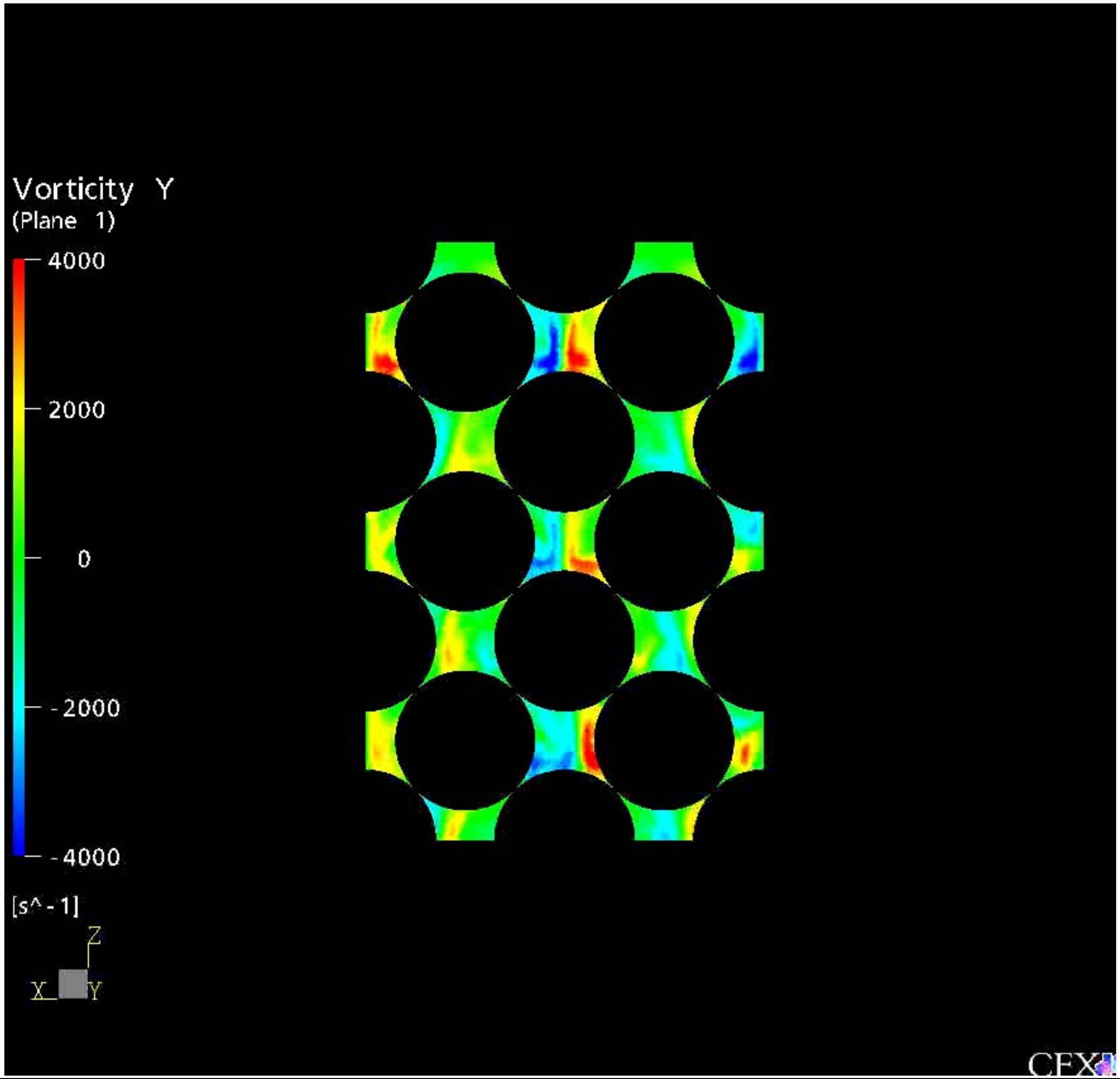
Vector Plot of Velocity Field



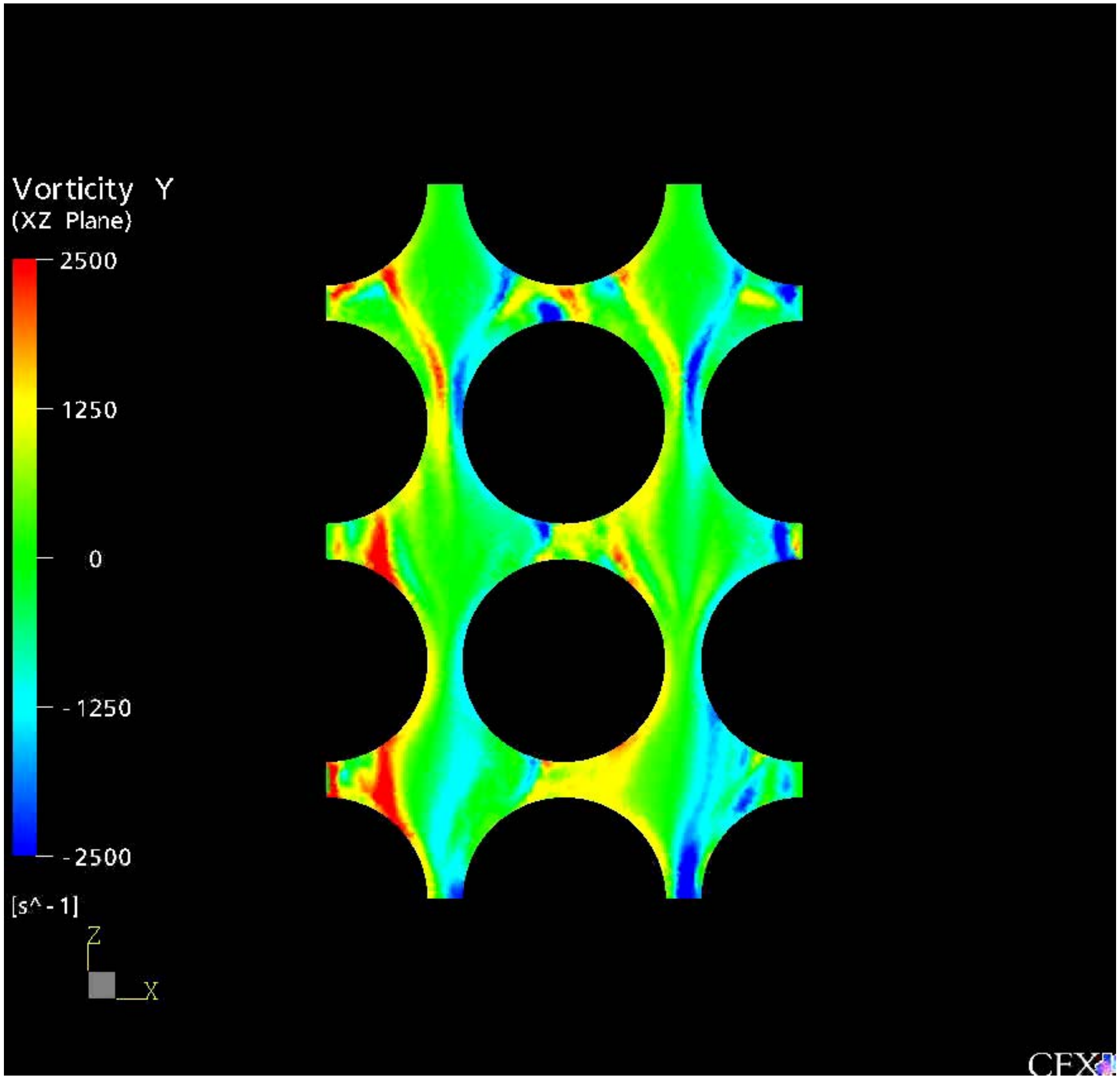
Vector Plot of Velocity Field at t=2.56 s (LES)



ω_y-Vorticity (Touching-Pebbles)



ω_y -Vorticity (Mid-Plane)

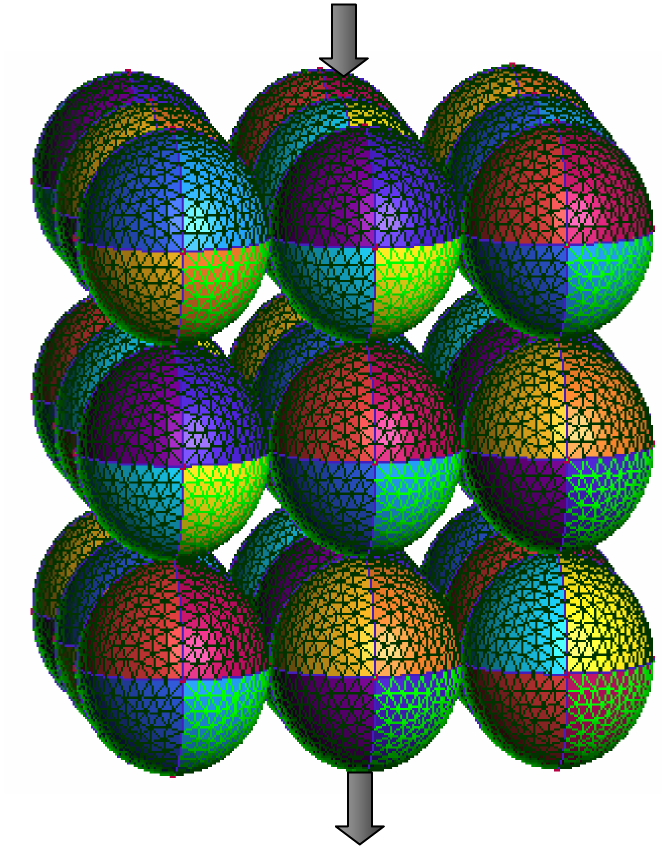


Flow in A Closed Packed Hot PBMR Core

In this part of the study, heat was added to the surface of the pebbles as in the case of PMBR. Behavior of flow field was investigated by adding thermal energy model to the simulations.

Turbulence Model	**Iteration range**	**Number of Iterations**	**RMS Mass and Momentum Residual**
Zero Equation	1-6	6	0.1473 %
Reynolds Stress	7-41	35	0.1473 %
Large Eddy Simulation	7-518	512	0.1473 %

SIMULATED GEOMETRY AND MESH GENERATION (Trio-U)



Continued…

- Calculations were performed using the CFD code Trio-U developed by French Atomic Agency (CEA).
- It is a thermo hydraulic calculation modular software including finite difference and finite element volume techniques.
- Central difference scheme was used for discretization of the equations in space. Second order Runge Kutta method was utilized for the discritization of equations in time.
- In this part of the study, spheres were arranged regularly.

CONCLUSIONS

- Two-phase bubbly flow is a complex and unpredictable.

- **Verification and Validation are the key to better predictions (accurate algorithms + Physics + Experiments)**